

MASH Native Installation Guide

Version 1.1

Overview

This document gives information on downloading and installing MASH Native Basic and its supporting software. Note that when you install supporting software, you need to use the Configuration dialog in MASH Native to specify where MASH Native should find the supporting software. Users can access the Configuration dialog via the Tools menu (Tools -> configuration). Boxes in the Configuration dialog (Figure 1) will appear green if the specified file path exists and red if it does not. If the dialog appears yellow, it means the directory exists, but the software cannot find the right executables. Use “Find” to automatically find supporting software, “Browse” to set the file path yourself, and “Download” to open the web page to download the corresponding software.

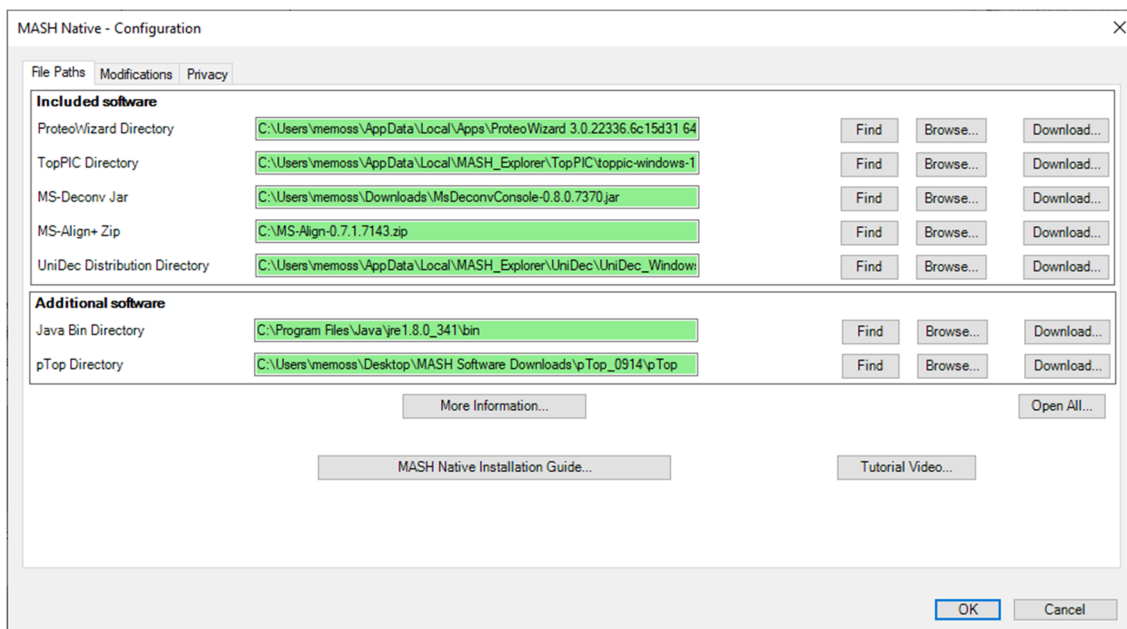


Figure 1. MASH Native configuration interface

Within the configuration interface, there are many resources to help configure and start using MASH Native. Within the dialog, there is the “MASH Native Installation Guide” button which will open documentation to help download the necessary software for users. On the right-hand side, the “Open All” button will open the links to download all included and additional software packages. Users will need to install the individual software packages if this is selected, then select the correct file path within the configuration dialog. The “More Information” button opens a document that explains to user the differences between required, included, and additional software. The “Tutorial Videos” button in the bottom right corner bring the users to multiple videos that introduce MASH Native, help with configuration, and give examples of Discovery and Targeted Mode workflows. It is important to note that Windows has a 270-character path limit. For this reason, all file paths to supporting software and raw data must be well below this limit, as MASH Native automatically creates new directories for your workflows within the folders containing the raw data for the workflow.

Software Package Download and Installation

The MASH Native software can be downloaded on our [website](#). After downloading the MASH Native.zip file, extract it into the folder where you would like to run MASH Native (Note: this should be a folder with a low path length). Before installing a new version of MASH Native, you need to uninstall any previous version you’ve installed (either MASH Explorer or MASH Native). You do not need to uninstall any of the supporting software to upgrade MASH Native itself. Then double-click the MASH `setup` file to install and run MASH Native. As of MASH Native version 1.1 release, MASH Native is now a signed software and should not require administrator access to download, regardless of a user’s home institution firewalls or security measures. However, a popup from Windows Defender may flag MASH Native as a potential security risk. If this is the case, select “Run Anyway” and the MASH Native installation will proceed normally.

Software algorithms

Many different software algorithms are compatible with MASH Native. The included software is fully supported by MASH Native and are included in the software package download. When users open the MASH Native application for the first time, the Welcome Screen (Figure 2) will pop-up and the UniDec and TopPIC Suite software packages will automatically begin to install on the user's computer. MASH Native will also prompt users to configure ProteoWizard, which is strongly recommended for optimal MASH Native function. Once the software is installed, users can select the *Go!* Button and begin using MASH Native (this button will be grey until UniDec and TopPIC Suite have successfully downloaded). For more information on the Welcome Screen, please refer to section 2 of the MASH Native User Manual.

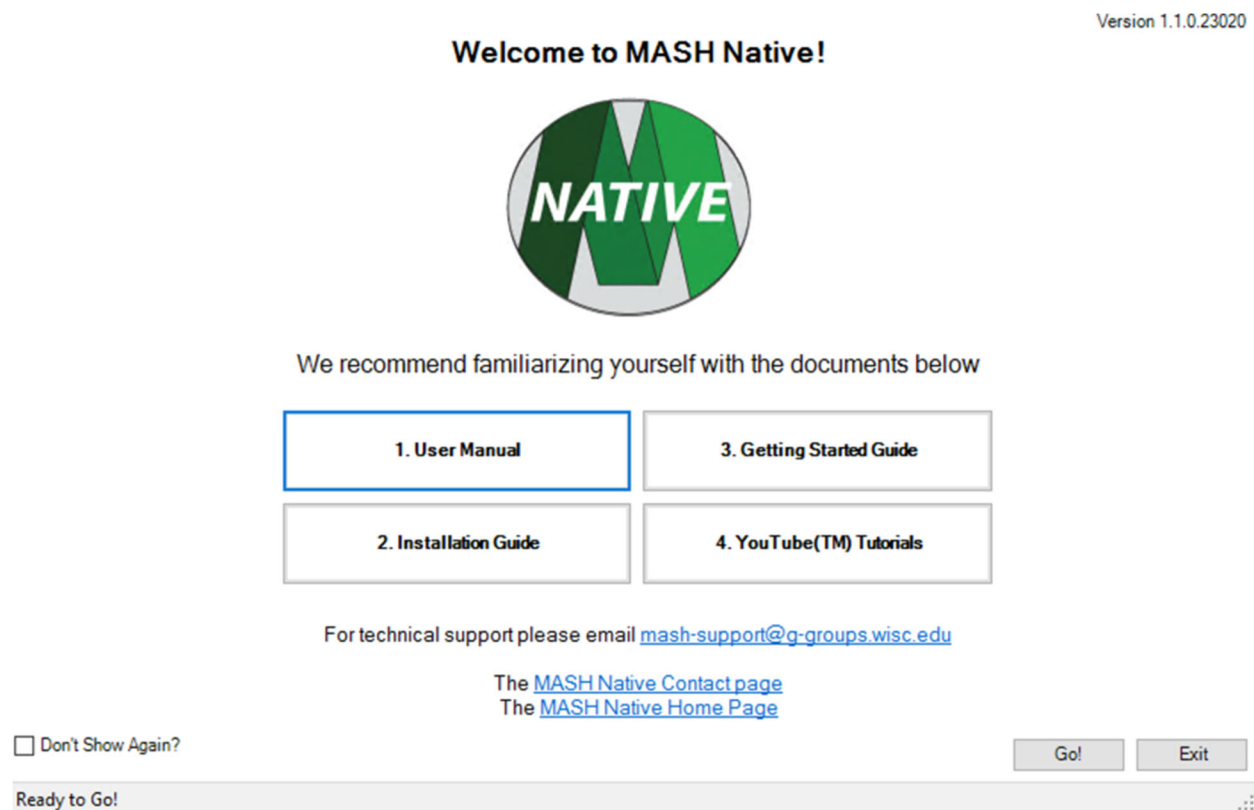


Figure 2. MASH Native Welcome screen

The Additional software algorithms are also supported by MASH Native and users can download them in addition to the included software, if they deem necessary. Additionally, we have

designated troubleshooting software that is available for download if users run into specific problems.

Required Software

1. Windows Operating System

MASH Native requires the Windows operating system and is currently not functional on other operating systems.

2. .NET Framework 3.5 SP1 and .NET Framework 4.8

MASH Native requires .NET Framework 4.8 or above and .NET Framework 3.5 SP1. .NET Framework 4.8 can be downloaded here: <https://dotnet.microsoft.com/download/dotnet-framework/net48>. The .NET Framework 3.5 SP1 can be downloaded here: <https://dotnet.microsoft.com/download/dotnet-framework/net35-sp1>. The user's computer must be connected to the internet in order to install these, or else they must be manually installed to run MASH Native.

Included Software

1. eTHRASH

MASH Native includes eTHRASH as a deconvolution algorithm within its software.

2. ProteoWizard, Windows 64-bit Installer

MASH Native has integrated ProteoWizard for convenient data import and data conversion. We strongly recommend installing ProteoWizard from the MASH Native welcome screen when prompted. If ProteoWizard is already on your computer, MASH Native will recognize it and configure it. ProteoWizard is not a requirement to run the MASH Native application, but it is a requirement to load most files into the application. ProteoWizard version v3.0.22198 is included in MASH Native.

3. MS-Deconv/MSAlign+

MASH Native includes a pre-configured version of MS-Deconv and MSAlign+ for deconvolution and database searching, respectively. MS-Deconv version 0.8.0.7370 and MSAlign+ version 0.7.1.7143 are included. **Please note that to use MS-Deconv or MSAlign+, 64-bit Java is required to install, using the link on page 5.** If using MS-Deconv or MSAlign+, please cite respective publications MS-Deconv (Mol Cell Proteomics 2010;9:2772-2782) and MSAlign+ (Mol Cell Proteomics 2012;11:M111.008524).

4. TopPIC Suite

MASH Native includes a version of TopPIC suite developed by Xiaowen Liu's research group in Indiana University – Purdue University Indianapolis. This software package includes TopFD, a deconvolution algorithm, and TopPIC, a database search algorithm. TopPIC Suite version 1.5.4 is included with MASH Native. When using the TopPIC algorithm for searching in MASH Native, please also acknowledge their paper (Bioinformatics, 32:3495-3497, 2016).

5. UniDec

MASH Native includes a version of UniDec developed by Michael Marty's research group in University of Arizona. UniDec can be run in interactive or non-interactive mode. In non-interactive mode, UniDec works within MASH Native automatically. In interactive mode, MASH Native launches UniDec with the relevant data already loaded. Users can manually process the data in UniDec and then it will be loaded back into MASH Native. UniDec version 5.0.5 is included with MASH Native. When using UniDec, please cite their publication (Anal. Chem. vol. 87, iss. 8, p. 4370-4376, 2015).

Additional Software

1. Java (64-bit)

To use MS-Deconv and MS-Align+, 64-bit Java needs to be installed on your computer. Java is not a requirement to run MASH Native, but it is a requirement to run MS-Deconv and MS-Align+ You can download the Java software with the following link <https://www.java.com/en/download/manual.jsp>. Download the Windows offline (64-bit version), as seen in Figure 3.



Figure 3. Java download interface

Follow the Java installation setup and copy Java into the following directory into the system drive shown below in Figure 4. Within the MASH Native configuration dialog, verify that the file path of the Java bin is correctly located (should match the path for the Java Bin Directory in figure 1).

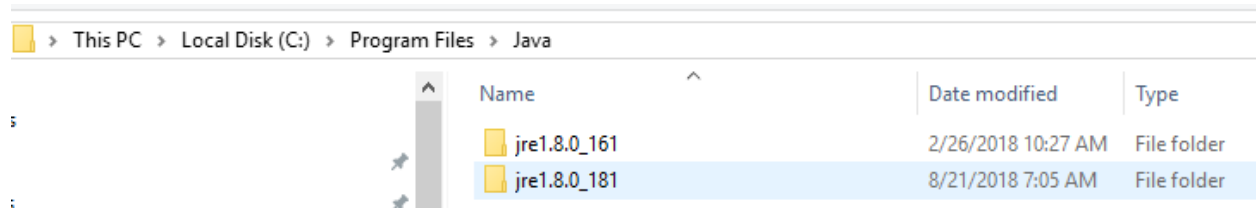


Figure 4. Java installation directory for MASH Native

2. pParseTD/pTop

Please use the following link to download pTop (<http://pfind.org/software/pTop/index.html>).

pParseTD is an embedded algorithm which is installed at the same time. Run the downloaded

executable file, pTop1.2_x64.exe (at the time of writing this document). Running pTop workflow will require installation of Xcalibur software. As with the Java Bin Directory, verify that the file path for pTop is correct in the MASH Native configuration dialog. When using this software package, please cite their publication (Anal. Chem., 2016, 88 (6), pp 3082–3090).

Troubleshooting Software from Vendors

1. Xcalibur 2.0.7+ or MSFileReader x64 or Thermo Data File Import

MASH Native and ProteoWizard are capable of reading Thermo .raw files on their own. In some cases, users may find themselves unable to do so. In this case, we recommend that Thermo users install either Xcalibur version 2.0.7 or above (please consult with your vendor regarding this software), or MSFileReader x64 (available from Thermo website upon account registration, <https://thermo.flexnetoperations.com/control/thmo/login?nextURL=%2Fcontrol%2Fthmo%2Fsearch%3Fquery%3DMSFileReader>). If your computer requires any administrative access when downloading applications select “Run as Administrator” when installing MSFileReader. Please download any version of MSFileReader except MSFileReader 3.1 SP4. Neither Xcalibur nor MSFileReader are required to run MASH Native but one or the other may be helpful in troubleshooting Thermo file parsing issues.

2. CompassXtract for Bruker data file import

Like the case in Thermo data import, sometimes MASH/ProteoWizard has trouble parsing some of the Bruker files. If trouble shooting is required, we recommend Bruker users install CompassXtract 64-bit (available from Bruker, <https://www.bruker.com/protected/en/services/software-downloads/mass-spectrometry/raw-data-access-libraries.html>; free registration needed). CompassXtract is not a requirement to run MASH Native but may be helpful in troubleshooting Bruker file parsing issues.